Gradient Descent

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February 5, 2019

Gradient Descent

Unconstrained Optimization

Setting

Objective function $f : \mathbf{R}^d \to \mathbf{R}$ is *differentiable.*
Want to find

$$x^* = \arg\min_{x \in \mathbf{R}^d} f(x)$$

The Gradient

- Let $f : \mathbf{R}^d \to \mathbf{R}$ be differentiable at $x_0 \in \mathbf{R}^d$.
- The **gradient** of f at the point x_0, denoted $\nabla_x f(x_0)$, is the direction to move in for the **fastest increase** in $f(x)$, when starting from x_0.

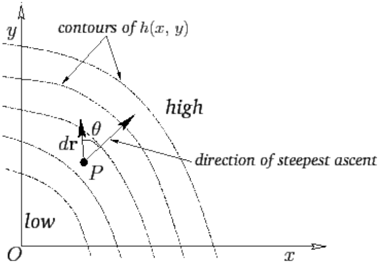


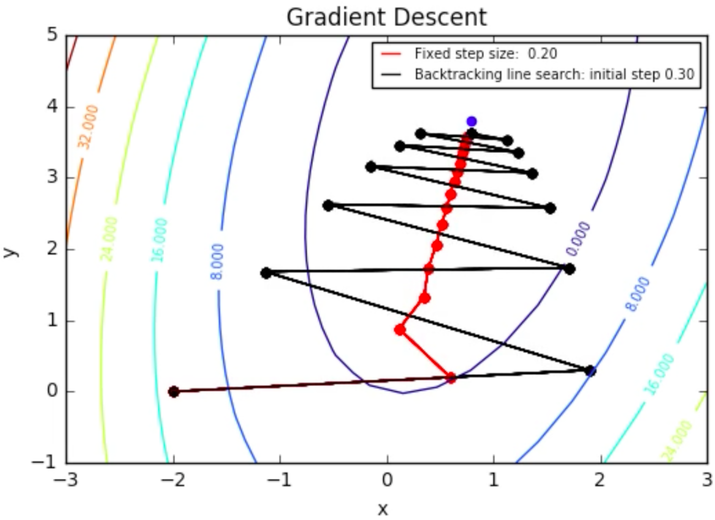
Figure A.111 from Newtonian Dynamics, by Richard Fitzpatrick.

Gradient Descent

Gradient Descent

- Initialize $x = 0$
- repeat
  - $x \leftarrow x - \underbrace{\eta}_{\text{step size}} \nabla f(x)$
- until stopping criterion satisfied

Gradient Descent Path



Gradient Descent: Step Size

- A fixed step size will work, eventually, as long as it's small enough (roughly - details to come)
    - Too fast, may diverge
    - In practice, try several fixed step sizes
- Intuition on when to take big steps and when to take small steps?

Convergence Theorem for Fixed Step Size

Theorem

Suppose $f : \mathbf{R}^d \to \mathbf{R}$ is convex and differentiable, and ∇f is ***Lipschitz continuous*** *with constant $L > 0$, i.e.*

$$\|\nabla f(x) - \nabla f(x')\| \leqslant L\|x - x'\|$$

for for any $x, x' \in \mathbf{R}^d$. Then gradient descent with fixed step size $\eta \leqslant 1/L$ ***converges****. In particular,*

$$f(x^{(k)}) - f(x^*) \leqslant \frac{\|x^{(0)} - x^*\|^2}{2\eta k}.$$

Step Size: Practical Note

- Although a $1/L$ step-size guarantees convergence,
    - it may be **much slower** than necessary.
- May be worth trying larger step sizes as well.
- But math tells us, no need for anything smaller.

Gradient Descent: When to Stop?

- Wait until $\|\nabla f(x)\|_2 \leqslant \varepsilon$, for some ε of your choosing.
  - (Recall $\nabla f(x) = 0$ at minimum.)
- For learning setting,
  - evalute performance on validation data as you go
  - stop when not improving, or getting worse